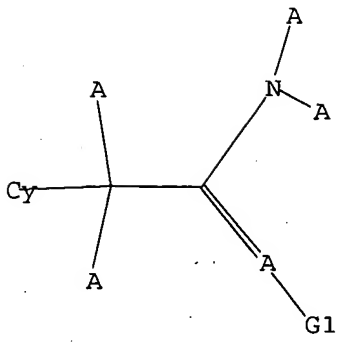


G1 CN,NO2

Structure attributes must be viewed using STN Express query preparation.

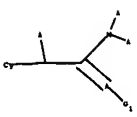
=> s l1 full
FULL SEARCH INITIATED 12:01:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1320267 TO ITERATE

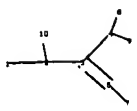
75.7% PROCESSED 1000000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.09

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1320267 TO 1320267
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS FUL L1

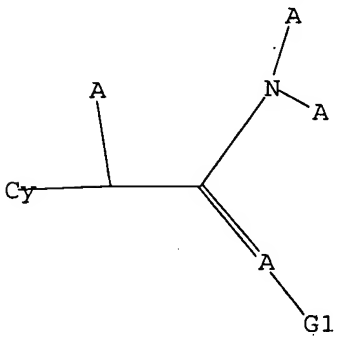
=>
Uploading C:\Program Files\Stnexp\Queries\10535653a.str



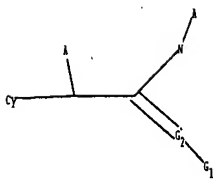


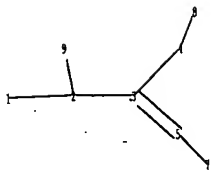
chain nodes :
1 5 7
ring/chain nodes :
2 3 4 8 9 10

```
chain bonds :
1-2  2-3  2-10  3-4  3-5  4-8  4-9  5-7
exact/norm bonds :
1-2  2-10  3-4  3-5  4-8  4-9  5-7
exact bonds :
2-3


G1:CN,NO2

Match level :
1:Atom  2:CLASS  3:CLASS  4:CLASS  5:CLASS  7:CLASS  8:CLASS  9:CLASS  10:CLASS



L3      STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3                STR
```




```
G1 CN,NO2


Structure attributes must be viewed using STN Express query preparation.


=> s l3 full
FULL SEARCH INITIATED 12:04:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  1343242 TO ITERATE

 74.4% PROCESSED  1000000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.09

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      1343242 TO  1343242
PROJECTED ANSWERS:               0 TO        0

L4             0 SEA SSS FUL L3

=>
Uploading C:\Program Files\Stnexp\Queries\10535653b.str
```





chain nodes :
1 5 7
ring/chain nodes :
2 3 4 8 9
chain bonds :
1-2 2-3 2-9 3-4 3-5 4-8 5-7
exact/norm bonds :
1-2 2-9 3-4 3-5 4-8 5-7
exact bonds :
2-3

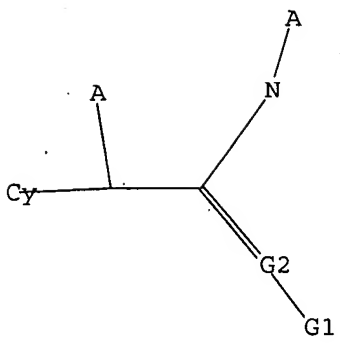
G1:CN,NO2

G2:C,N,P,CS2H,CSSH,CHO,C(O)CH3,NH,NH2,A,Ak

Hydrogen count :
2:>= minimum 0 4:>= minimum 0
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS 9:CLASS

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



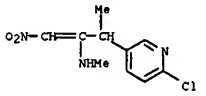
G1 CN,NO2

G2 C,N,P,CS2H,CSSH,CHO,C(O)CH3,NH,NH2,A,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> s l5 full
FULL SEARCH INITIATED 12:11:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  2872067 TO ITERATE

 34.8% PROCESSED  1000000 ITERATIONS                                29 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.17

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      2872067 TO  2872067
PROJECTED ANSWERS:              56 TO      110

L6            29 SEA SSS FUL L5

=> d l6 1-15
```

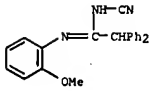
L6 ANSWER 1 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 938069-24-0 REGISTRY
ED Entered STN: 20 Jun 2007
CN 3-Pyridineethanamine, 6-chloro-N,β-dimethyl-α-(nitromethylene)-
(CA INDEX NAME)
MF C10 H12 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

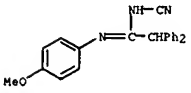
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 2 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 907166-58-9 REGISTRY
ED Entered STN: 17 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C22 H19 N3 O
SR Other Sources
Database: NCI 3D (National Cancer Institute)



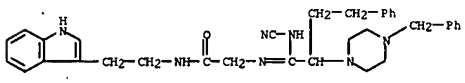
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L6 ANSWER 3 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 906638-56-0 REGISTRY
ED Entered STN: 14 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C22 H19 N3 O
SR Other Sources
Database: NCI 3D (National Cancer Institute)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

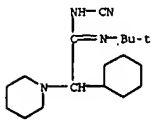
L6 ANSWER 4 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-94-2 REGISTRY
ED Entered STN: 27 Apr 2006
CN Acetamide, 2-[[1-(cyanoamino)-4-phenyl-2-[4-(phenylmethyl)-1-
piperazinyl]butylidene]amino]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)
MF C34 H39 N7 O
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

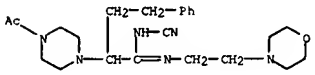
L6 ANSWER 5 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-93-1 REGISTRY
ED Entered STN: 27 Apr 2006
CN 1-Piperidineethanimidamide, N-cyano-α-cyclohexyl-N'-(1,1-dimethylethyl)- (CA INDEX NAME)
MF C18 H32 N4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

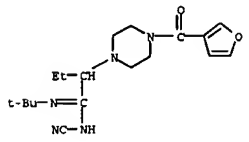
L6 ANSWER 6 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-92-0 REGISTRY
ED Entered STN: 27 Apr 2006
CN 1-Piperazineethanimidamide, 4-acetyl-N-cyano-N'-[2-(4-morpholinyl)ethyl]-α-(2-phenylethyl)- (CA INDEX NAME)
MF C23 H34 N6 O2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

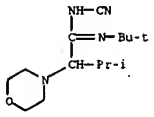
L6 ANSWER 7 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-91-9 REGISTRY
ED Entered STN: 27 Apr 2006
CN 1-Piperazineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-ethyl-4-(3-furanylcarbonyl)- (CA INDEX NAME)
MF C18 H27 N5 O2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

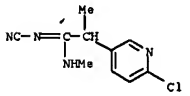
L6 ANSWER 8 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-90-8 REGISTRY
ED Entered STN: 27 Apr 2006
CN 4-Morpholineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-(1-methylethyl)- (CA INDEX NAME)
MF C14 H26 N4 O
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 9 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717913-05-8 REGISTRY
ED Entered STN: 28 Jul 2004
CN 3-Pyridineethanimidamide, 6-chloro-N'-cyano-N,α-dimethyl-, [C(Z)]-(9CI) (CA INDEX NAME)
MF C10 H11 Cl N4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

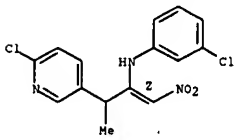


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 10 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717106-64-4 REGISTRY
ED Entered STN: 27 Jul 2004
CN 3-Pyridineethanamine, 6-chloro-N-(3-chlorophenyl)-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H13 Cl2 N3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

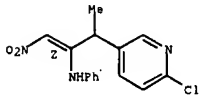


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 11 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717106-62-2 REGISTRY
ED Entered STN: 27 Jul 2004
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-phenyl-, (αZ)- (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H14 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

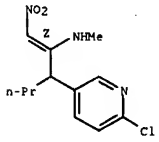


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 12 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717106-60-0 REGISTRY
ED Entered STN: 27 Jul 2004
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-propyl-, (αZ)- (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H16 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

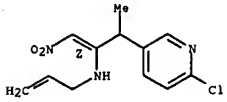


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 13 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717106-56-4 REGISTRY
ED Entered STN: 27 Jul 2004
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-2-propenyl-, (αZ)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H14 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

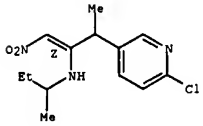


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 14 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717106-55-3 REGISTRY
ED Entered STN: 27 Jul 2004
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(1-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H18 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.

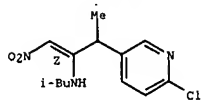


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 15 OF 29 REGISTRY COPYRIGHT 2008 ACS on STN
RN 717106-53-1 REGISTRY
ED Entered STN: 27 Jul 2004
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(2-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H18 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	572.90	574.37

FILE 'CAPLUS' ENTERED AT 12:13:12 ON 04 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 4 Jan 2008 VOL 148 ISS 2
FILE LAST UPDATED: 3 Jan 2008 (20080103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

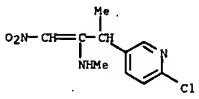
=> s l6

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:644247 CAPLUS
DOCUMENT NUMBER: 147:25346
TITLE: Activity enhancement of neonicotinoid insecticides by ammonium or phosphonium compounds
INVENTOR(S): Jeschke, Peter; Nauen, Ralf; Pontzen, Rolf; Reckmann, Udo; Marczok, Peter; Fischer, Reiner; Velten, Robert; Arnold, Christian; Sanwald, Erich
PATENT ASSIGNEE(S): Bayer Cropscience A.-G., Germany
SOURCE: Ger. Offen., 22pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

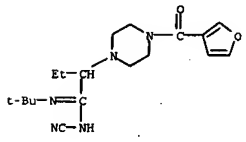
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102005059468	A1	20070614	DE 2005-102005059468	20051213
WO 2007068355	A1	20070621	WO 2006-EP11468	20061130

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

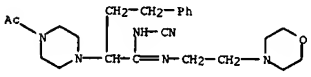
PRIORITY APPLN. INFO.: DE 2005-102005059468A 20051213
AB The insecticidal activity of inhibitors of nicotinergic acetylcholine receptors (for example neonicotinoids) is enhanced by addition of ammonium or phosphonium salts or quaternary ammonium salts and/or quaternary phosphonium salts. Penetration promoters, such as fatty alc. ethoxylates and mineral or vegetable oil esters, further enhance the activity.
IT 938069-24-0D, mixts. with (quaternary) ammonium or phosphonium salts
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(insecticides with enhanced activity)
RN 938069-24-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N,β-dimethyl-α-(nitromethylene)- (CA INDEX NAME)



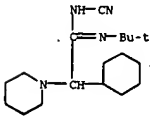
L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



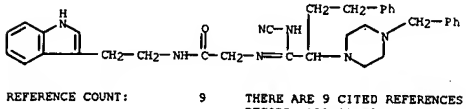
RN 882006-92-0 CAPLUS
CN 1-Piperazineethanimidamide, 4-acetyl-N-cyano-N'-[2-(4-morpholinyl)ethyl]-α-(2-phenylethyl)- (CA INDEX NAME)



RN 882006-93-1 CAPLUS
CN 1-Piperidineethanimidamide, N-cyano-α-cyclohexyl-N'-(1,1-dimethylethyl)- (CA INDEX NAME)

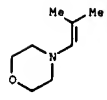


RN 882006-94-2 CAPLUS
CN Acetamide, 2-[[1-(cyanoamino)-4-phenyl-2-[4-(phenylmethyl)-1-piperazinyl]butylidene]amino]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)

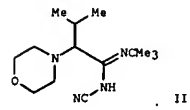


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:128444 CAPLUS
DOCUMENT NUMBER: 144:369409
TITLE: Cyanamide in isocyanide-based MCRs
AUTHOR(S): Doemling, Alexander; Herdtweck, Eberhardt; Heck, Stefan
CORPORATE SOURCE: ABC Pharma, Munich, 81243, Germany
SOURCE: Tetrahedron Letters (2006), 47(11), 1745-1747
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369409
GI

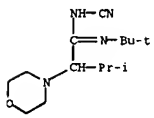


I



II

AB Cyanamide reacts with enamines and isocyanides in the presence of Lewis acids to give the hitherto unknown scaffold 2-amino-(N-cyano)-amidines. Preliminary scope and limitation of this novel reaction is described. E.g., reaction of enamine I, Me3CNC, and cyanamide in MeOH gave 65% 2-amino-(N-cyano)-amidine II.
IT 882006-90-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-amino-(N-cyano)-amidines by reaction of cyanamide with enamines and isocyanides)
RN 882006-90-8 CAPLUS
CN 4-Morpholineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-(1-methylethyl)- (CA INDEX NAME)



IT 882006-91-9P 882006-92-0P 882006-93-1P
882006-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-amino-(N-cyano)-amidines by reaction of cyanamide with enamines and isocyanides)
RN 882006-91-9 CAPLUS
CN 1-Piperazineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-ethyl-4-(3-furanylcarbonyl)- (CA INDEX NAME)

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:566527 CAPLUS
DOCUMENT NUMBER: 141:101553
TITLE: Preparation of insecticidal, acaricidal and nematocidal pyridine derivatives
INVENTOR(S): Benko, Zoltan Laszlo; Deamicis, Carl Vincent; Demeter, David Anthony; Markley, Lowell Dean; Samaritoni, Jack Geno; Schmidt, Carrie Lynn Rau; Zhu, Yuamning; Erickson, W. Randal; Anzeveno, Peter Biagio; Pechacek, James Todd; Watson, Gerald Bryan; Deboer, Gerrit Jan; Sheets, Joel Jay; Zabik, Susan Erhardt; Yerkes, Carla Nanette; Schobert, Christian Thomas; Dripps, James Edwin; Dintenfass, Leonard Paul; Karr, Laura Lee; Neese, Paul Allen; Huang, Jim Xinpei; Gifford, James Michael
PATENT ASSIGNEE(S): Dow Agrosciences LLC, USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004057960	A2	20040715	WO 2003-US41067	20031219
WO 2004057960	A3	20041104		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003303336	A1	20040722	AU 2003-303336	20031219
EP 1572656	A2	20050914	EP 2003-808550	20031219

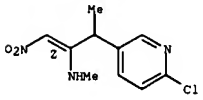
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

US 2006063741	A1	20060323	US 2005-535653	20050519

PRIORITY APPLN. INFO.: US 2002-435928P P 20021220
WO 2003-US41067 W 20031219
OTHER SOURCE(S): MARPAT 141:101553
AB The compds. QCR1R2C(:XZ)NR3R4 [Q = carbocyclyl or heterocyclyl, preferably pyridyl; X = N, CR, COR, CSOnR; CNR2, etc.; R1-5 = (cyclo)alkyl, (cyclo)alkenyl, alkoxy, aryl, etc.; n = 0, 1 or 2; Z = CN or NO2; R1CR2 = carbocyclyl or heterocyclyl] are prepared as insecticide, acaricide or nematocides.
IT 717106-21-3P 717106-24-6P 717106-25-7P
717106-28-0P 717106-32-6P 717106-33-7P
717106-37-1P 717106-38-2P 717106-39-3P
717106-42-8P 717106-45-1P 717106-46-2P
717106-48-4P 717106-51-9P 717106-53-1P
717106-55-3P 717106-56-4P 717106-60-0P
717106-62-2P 717106-64-4P 717913-05-8P
RL: AGR (Agricultural use); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as insecticide, acaricide and nematocides)

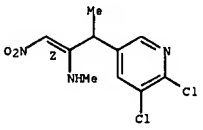
RN 717106-21-3 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N,β-dimethyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



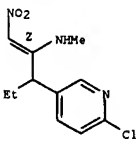
RN 717106-24-6 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-N,β-dimethyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 717106-25-7 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-ethyl-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

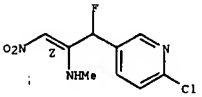
Double bond geometry as shown.



RN 717106-28-0 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-N-ethyl-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

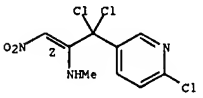
Double bond geometry as shown.

Double bond geometry as shown.



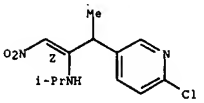
RN 717106-39-3 CAPLUS
CN 3-Pyridineethanamine, β,β,6-trichloro-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



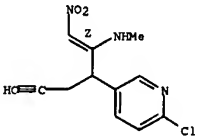
RN 717106-42-8 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(1-methylethyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

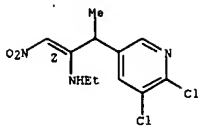
Double bond geometry as shown.



RN 717106-45-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-2-propynyl-, (αZ)- (9CI) (CA INDEX NAME)

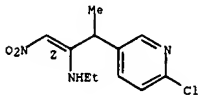
Double bond geometry as shown.





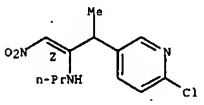
RN 717106-32-6 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-ethyl-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



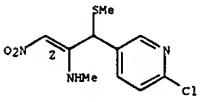
RN 717106-33-7 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 717106-37-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-β-(methylthio)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

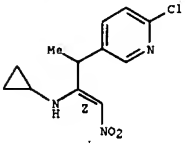
Double bond geometry as shown.



RN 717106-38-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-fluoro-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

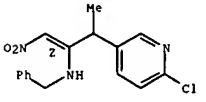
RN 717106-46-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-cyclopropyl-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



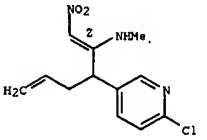
RN 717106-48-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-(phenylmethyl)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



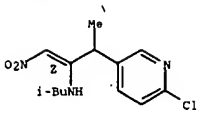
RN 717106-51-9 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-2-propenyl-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



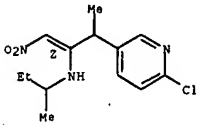
RN 717106-53-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(2-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



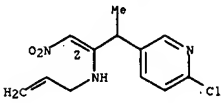
RN 717106-55-3 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(1-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



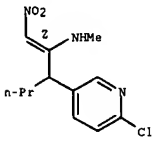
RN 717106-56-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-2-propenyl-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



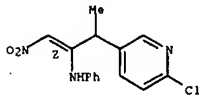
RN 717106-60-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



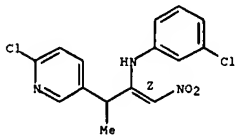
RN 717106-62-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-phenyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

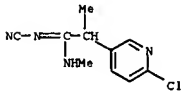


RN 717106-64-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(3-chlorophenyl)-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 717913-05-8 CAPLUS
CN 3-Pyridineethanimidamide, 6-chloro-N'-cyano-N,α-dimethyl-, [C(Z)]-(9CI) (CA INDEX NAME)



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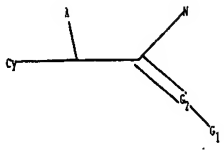
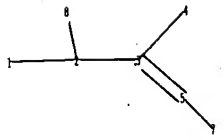




chain nodes :
1 5 7
ring/chain nodes :
2 3 4 8
chain bonds :
1-2 2-3 2-8 3-4 3-5 5-7
exact/norm bonds :
1-2 2-8 3-4 3-5 5-7
exact bonds :
2-3

G1:CN,NO2

G2:C,N,P,CS2H,CSSH,CHO,C(O)CH3,NH,NH2,A,Ak

Hydrogen count :
2:>= minimum 0 4:>= minimum 0
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS 8:CLASS

L8 STRUCTURE UPLOADED

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	19.71	594.08

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.40	-2.40

FILE 'REGISTRY' ENTERED AT 12:17:10 ON 04 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 3 JAN 2008 HIGHEST RN 959958-02-2
DICTIONARY FILE UPDATES: 3 JAN 2008 HIGHEST RN 959958-02-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

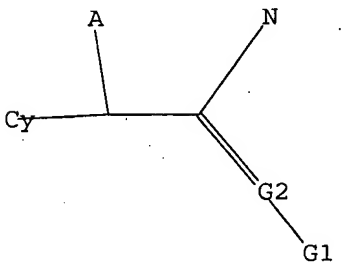
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d l8
L8 HAS NO ANSWERS
L8 STR



G1 CN,NO2

G2 C,N,P,CS2H,CSSH,CHO,C(O)CH3,NH,NH2,A,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l8 full
FULL SEARCH INITIATED 12:17:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2873949 TO ITERATE

34.8% PROCESSED 1000000 ITERATIONS 33 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.17

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2873949 TO 2873949
PROJECTED ANSWERS: 65 TO 123

L9 33 SEA SSS FUL L8

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.36	772.44

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.40

FILE 'CAPLUS' ENTERED AT 12:17:42 ON 04 JAN 2008
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FILE LAST UPDATED: 3 Jan 2008 (20080103/ED)

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=> s l9
L10 4 L9

=> d l10 1-4 ibib abs

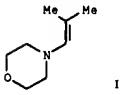
L10 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:644247 CAPLUS
DOCUMENT NUMBER: 147:25346
TITLE: Activity enhancement of neonicotinoid insecticides by ammonium or phosphonium compounds
INVENTOR(S): Jeschke, Peter; Nauen, Ralf; Pontzen, Rolf; Reckmann, Udo; Marczok, Peter; Fischer, Reiner; Velten, Robert; Arnold, Christian; Sanwald, Erich
PATENT ASSIGNEE(S): Bayer Cropscience A.-G., Germany
SOURCE: Ger. Offen., 22pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102005059468	A1	20070614	DE 2005-102005059468	20051213
WO 2007068355	A1	20070621	WO 2006-EP11468	20061130

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2005-102005059468A 20051213
AB The insecticidal activity of inhibitors of nicotinergic acetylcholine receptors (for example neonicotinoids) is enhanced by addition of ammonium or phosphonium salts or quaternary ammonium salts and/or quaternary phosphonium salts. Penetration promoters, such as fatty alc. ethoxylates and mineral or vegetable oil esters, further enhance the activity.

L10 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:128444 CAPLUS
DOCUMENT NUMBER: 144:369409
TITLE: Cyanamide in isocyanide-based MCRs
AUTHOR(S): Doemling, Alexander; Herdtweck, Eberhardt; Hack, Stefan
CORPORATE SOURCE: ABC Pharma, Munich, 81243, Germany
SOURCE: Tetrahedron Letters (2006), 47(11), 1745-1747
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369409
GI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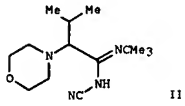

II

AB Cyanamide reacts with enamines and isocyanides in the presence of Lewis acids to give the hitherto unknown scaffold 2-amino-(N-cyano)-amidines. Preliminary scope and limitation of this novel reaction is described. E.g., reaction of enamine I, Me3CNC, and cyanamide in MeOH gave 65% 2-amino-(N-cyano)-amidine II.
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:359325 CAPLUS
DOCUMENT NUMBER: 144:88091
TITLE: Cyanoacetylene and its derivatives. Part XXXII. Addition of ammonia and methylamine to 4-hydroxy-4,4-diphenyl-2-butynenitrile
AUTHOR(S): Mal'kina, A. G.; Sokolyanskaya, L. V.; Kudyakova, R. N.; Sinegovskaya, L. M.; Albanov, A. I.; Shemyakina, O. A.; Trofimov, B. A.
CORPORATE SOURCE: Favorskii Irkutsk Institute of Chemistry, Siberian Division, Russian Academy of Sciences, Irkutsk, 664033, Russia
SOURCE: Russian Journal of Organic Chemistry (2005), 41(1), 61-66
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: Pleiades Publishing, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:88091
AB Nucleophilic addition of 25% aqueous NH3 and MeNH2 to 4-hydroxy-4,4-diphenyl-2-butynenitrile occurs under mild conditions to afford 4-amino- or 4-methylamino-2,5-dihydro-5,5-diphenyl-2-iminofurans. 4-Hydroxy-4,4-diphenyl-2-butynenitrile in anhydrous liquid NH3 gives rise to 3-amino-4-hydroxy-4,4-diphenyl-2-butenenitrile which is quant. converted into the corresponding iminodihydrofuran or iminodihydrofuran.HCl in the presence of 10 wt% of KOH or gaseous HCl. 4-Amino- and 4-methylamino-2-iminofurans react with 4-hydroxy-4-methyl-2-pentynenitrile to give 3-(4-amino- and 4-methylamino-5,5-diphenyl-2,5-dihydrofuran-2-ylideneamino)-4-hydroxy-4-methyl-2-pentenenitriles.
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:566527 CAPLUS
DOCUMENT NUMBER: 141:101553
TITLE: Preparation of insecticidal, acaricidal and nematocidal pyridine derivatives
INVENTOR(S): Benko, Zoltan Laszlo; Deamicis, Carl Vincent; Demeter, David Anthony; Markley, Lowell Dean; Samaritoni, Jack Geno; Schmidt, Carrie Lynn Rau; Zhu, Yuamning; Erickson, W. Randal; Anzeveno, Peter Biagio; Pechacek, James Todd; Watson, Gerald Bryan; Deboer, Gerrit Jan; Sheets, Joel Jay; Zabik, Susan Erhardt; Yerkes, Carla Nanette; Schobert, Christian Thomas; Dripps, James Edwin; Dintenfass, Leonard Paul; Karr, Laura Lee; Neese, Paul Allen; Huang, Jim Xinpei; Gifford, James Michael
PATENT ASSIGNEE(S): Dow Agrosciences LLC, USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004057960	A2	20040715	WO 2003-US41067	20031219
WO 2004057960	A3	20041104		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003303336	A1	20040722	AU 2003-303336	20031219
EP 1572656	A2	20050914	EP 2003-808550	20031219

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

US 2006063741	A1	20060323	US 2005-535653	20050519

PRIORITY APPLN. INFO.: US 2002-435928P P 20021220
WO 2003-US41067 W 20031219
OTHER SOURCE(S): MARPAT 141:101553
AB The compds. QCR1R2C(:XZ)NR3R4 [Q = carbocyclyl or heterocyclyl, preferably pyridyl; X = N, CR, COR, CSOnR; CNR2, etc.; R1-5 = (cyclo)alkyl, (cyclo)alkenyl, alkoxy, aryl, etc.; n = 0, 1 or 2; Z = CN or NO2; R1CR2 = carbocyclyl or heterocyclyl] are prepared as insecticide, acaricide or nematocides.

2 3 4
chain bonds :
1-2 2-3 3-4 3-5 5-7
exact/norm bonds :
1-2 3-4 3-5 5-7
exact bonds :
2-3

G1:CN,NO2

G2:C,N,P,CS2H,CSSH,CHO,C(O)CH3,NH,NH2,A,Ak

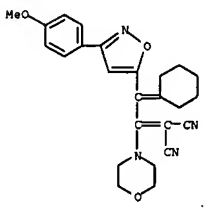
Hydrogen count :
2:>= minimum 0 4:>= minimum 0
Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 7:CLASS

L11   STRUCTURE UPLOADED

=> d
L11 HAS NO ANSWERS
L11   STR

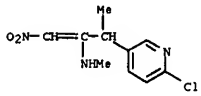
=> d l12 1-20

L12 ANSWER 1 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 959309-41-2 REGISTRY
ED Entered STN: 21 Dec 2007
CN INDEX NAME NOT YET ASSIGNED
MF C25 H26 N4 O3
SR Other Sources
Database: NIST Mass Spectral Library (National Institute of Standards and Technology)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 2 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 938069-24-0 REGISTRY
ED Entered STN: 20 Jun 2007
CN 3-Pyridineethanamine, 6-chloro-N,β-dimethyl-α-(nitromethylene)- (CA INDEX NAME)
MF C10 H12 Cl N3 O2
SR CA
LC STN Files: CA, CAPLUS

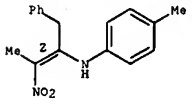


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 3 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 936102-78-2 REGISTRY
ED Entered STN: 30 May 2007
CN Benzeneethanamine, N-(4-methylphenyl)-α-(1-nitroethylidene)-, (αZ)- (CA INDEX NAME)
FS STEREOSEARCH
MF C17 H18 N2 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT

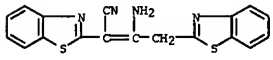
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

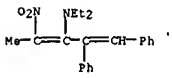
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 4 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 930421-15-1 REGISTRY
ED Entered STN: 17 Apr 2007
CN 2-Benzothiazoleacetonitrile, α-[1-amino-2-(2-benzothiazolyl)ethylidene]- (CA INDEX NAME)
MF C18 H12 N4 S2
SR Chemical Library
Supplier: Enamine
LC STN Files: CHEMCATS



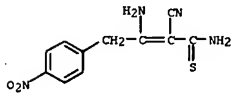
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 5 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 911810-16-7 REGISTRY
ED Entered STN: 01 Nov 2006
CN INDEX NAME NOT YET ASSIGNED
MF C21 H24 N2 O2
SR Other Sources
Database: Wiley Subscription Services, Inc.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

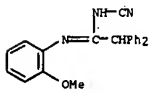
L12 ANSWER 6 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 909028-97-3 REGISTRY
ED Entered STN: 28 Sep 2006
CN 2-Butenethioamide, 3-amino-2-cyano-4-(4-nitrophenyl)- (CA INDEX NAME)
MF C11 H10 N4 O2 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

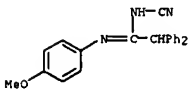
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 7 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 907166-58-9 REGISTRY
ED Entered STN: 17 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C22 H19 N3 O
SR Other Sources
Database: NCI 3D (National Cancer Institute)



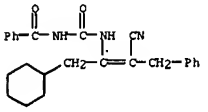
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 8 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 906638-56-0 REGISTRY
ED Entered STN: 14 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
MF C22 H19 N3 O
SR Other Sources
Database: NCI 3D (National Cancer Institute)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

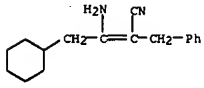
L12 ANSWER 9 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 883854-15-7 REGISTRY
ED Entered STN: 11 May 2006
CN Benzamide, N-[[[2-cyano-1-(cyclohexylmethyl)-3-phenyl-1-propenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)
MF C25 H27 N3 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

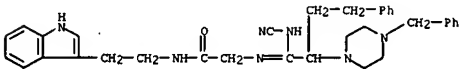
L12 ANSWER 10 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 883854-05-5 REGISTRY
ED Entered STN: 11 May 2006
CN Benzenepropanenitrile, α-(1-amino-2-cyclohexylethylidene)- (CA INDEX NAME)
MF C17 H22 N2
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

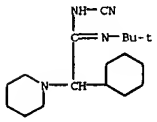
L12 ANSWER 11 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-94-2 REGISTRY
ED Entered STN: 27 Apr 2006
CN Acetamide, 2-[[1-(cyanoamino)-4-phenyl-2-[4-(phenylmethyl)-1-piperazinyl]butylidene]amino]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)
MF C34 H39 N7 O
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

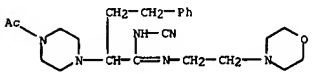
L12 ANSWER 12 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-93-1 REGISTRY
ED Entered STN: 27 Apr 2006
CN 1-Piperidineethanimidamide, N-cyano-α-cyclohexyl-N'-(1,1-dimethylethyl)- (CA INDEX NAME)
MF C18 H32 N4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

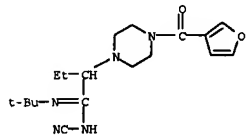
L12 ANSWER 13 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-92-0 REGISTRY
ED Entered STN: 27 Apr 2006
CN 1-Piperazineethanimidamide, 4-acetyl-N-cyano-N'-[2-(4-morpholinyl)ethyl]-α-(2-phenylethyl)- (CA INDEX NAME)
MF C23 H34 N6 O2
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 14 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-91-9 REGISTRY
ED Entered STN: 27 Apr 2006
CN 1-Piperazineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-ethyl-4-(3-furanylcarbonyl)- (CA INDEX NAME)
MF C18 H27 N5 O2
SR CA
LC STN Files: CA, CAPLUS



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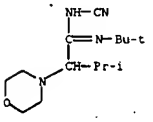
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 15 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 882006-90-8 REGISTRY
ED Entered STN: 27 Apr 2006
CN 4-Morpholineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-(1-methylethyl)- (CA INDEX NAME)
MF C14 H26 N4 O
SR CA
LC STN Files: CA, CAPLUS, CASREACT



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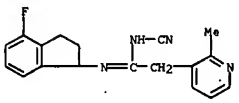
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 16 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 874993-89-2 REGISTRY
ED Entered STN: 23 Feb 2006
CN 3-Pyridineethanimidamide, N-cyano-N'-(4-fluoro-2,3-dihydro-1H-inden-1-yl)-2-methyl- (CA INDEX NAME)
MF C18 H17 F N4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



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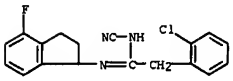
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

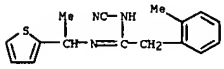
L12 ANSWER 17 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 874993-88-1 REGISTRY
ED Entered STN: 23 Feb 2006
CN Benzeneethanimidamide, 2-chloro-N-cyano-N'-(4-fluoro-2,3-dihydro-1H-inden-1-yl)- (CA INDEX NAME)
MF C18 H15 Cl F N3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

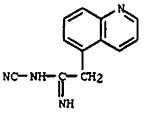
L12 ANSWER 18 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 874993-87-0 REGISTRY
ED Entered STN: 23 Feb 2006
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[1-(2-thienyl)ethyl]- (CA INDEX NAME)
MF C16 H17 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

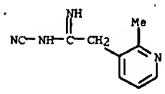
L12 ANSWER 19 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 874993-75-6 REGISTRY
ED Entered STN: 23 Feb 2006
CN 5-Quinolineethanimidamide, N-cyano- (CA INDEX NAME)
MF C12 H10 N4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L12 ANSWER 20 OF 159 REGISTRY COPYRIGHT 2008 ACS on STN
RN 874993-73-4 REGISTRY
ED Entered STN: 23 Feb 2006
CN 3-Pyridineethanimidamide, N-cyano-2-methyl- (CA INDEX NAME)
MF C9 H10 N4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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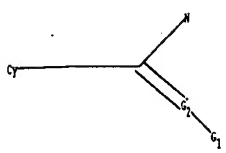
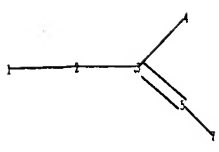
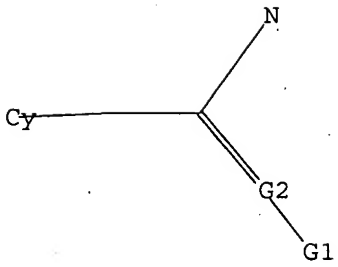
Uploading C:\Program Files\Stnexp\Queries\10535653e.str





chain nodes :
1 5 7
ring/chain nodes :
2 3 4
chain bonds :
1-2 2-3 3-4 3-5 5-7
exact/norm bonds :
1-2 3-4 3-5 5-7



G1 CN,NO2

G2 C,N,P,CS2H,CSSH,CHO,C(O)CH3,A,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l13 full
FULL SEARCH INITIATED 12:21:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2874351 TO ITERATE

34.4% PROCESSED 987583 ITERATIONS 157 ANSWERS

34.8% PROCESSED 1000000 ITERATIONS 159 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.16

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

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FILE COVERS 1907 - 4 Jan 2008 VOL 148 ISS 2
FILE LAST UPDATED: 3 Jan 2008 (20080103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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http://www.cas.org/infopolicy.html

=> s l14
L15   12 L14

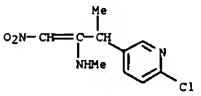
=> d l15 1-12 ibib abs hitstr

L15 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:644247 CAPLUS
DOCUMENT NUMBER: 147:25346
TITLE: Activity enhancement of neonicotinoid insecticides by ammonium or phosphonium compounds
INVENTOR(S): Jeschke, Peter; Nauen, Ralf; Pontzen, Rolf; Reckmann, Udo; Marczok, Peter; Fischer, Reiner; Velten, Robert; Arnold, Christian; Sanwald, Erich
PATENT ASSIGNEE(S): Bayer Cropscience A.-G., Germany
SOURCE: Ger. Offen., 22pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102005059468	A1	20070614	DE 2005-102005059468	20051213
WO 2007068355	A1	20070621	WO 2006-EP11468	20061130

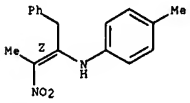
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: DE 2005-102005059468A 20051213
AB The insecticidal activity of inhibitors of nicotinergic acetylcholine receptors (for example neonicotinoids) is enhanced by addition of ammonium or phosphonium salts or quaternary ammonium salts and/or quaternary phosphonium salts. Penetration promoters, such as fatty alc. ethoxylates and mineral or vegetable oil esters, further enhance the activity.
IT 938069-24-0D, mixts. with (quaternary) ammonium or phosphonium salts
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(insecticides with enhanced activity)
RN 938069-24-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N,β-dimethyl-α-(nitromethylene)- (CA INDEX NAME)



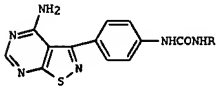
L15 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:194096 CAPLUS
DOCUMENT NUMBER: 146:500589
TITLE: C-imidoylation of esters, sulfones, sulfoxides, amides and nitro compounds
AUTHOR(S): Katritzky, Alan R.; Khashab, Niveen M.; Singh, Anamika
CORPORATE SOURCE: Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: ARKIVOC (Gainesville, FL, United States) (2007), (5), 263-276
CODEN: AGFUAR
URL: http://content.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2007/LT-2249HP%20as%20published%20mainmanuscript.pdf
PUBLISHER: Arkat USA Inc.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:500589
AB C-Imidoylation of esters, sulfones, sulfoxides, amides, and nitro- compds. with N-imidoylbenzotriazoles gave β-enamino esters, β-imino sulfones, β-enamino sulfoxides, β-imino amides, and α-nitro enamines resp. in good yields. Strong electron-withdrawing substitutes (esters, sulfoxides, nitroethane) tended to give enamines due to increased acidity of the α-protons, while weak electron-withdrawing substitutes(sulfones, amides) gave imines instead.
IT 936102-78-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of enamino esters, sulfoxides, imino sulfones, amides, nitroenamines via condensation of benzotriazole with amides followed by imidoylation of alkanoates, sulfones, sulfoxides, phenylacetamide or nitroethane)
RN 936102-78-2 CAPLUS
CN Benzeneethanamine, N-(4-methylphenyl)-α-(1-nitroethylidene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



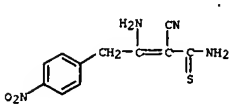
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:693859 CAPLUS
DOCUMENT NUMBER: 145:314939
TITLE: Isothiazolopyrimidines and isoxazolopyrimidines as novel multi-targeted inhibitors of receptor tyrosine kinases
AUTHOR(S): Ji, Zhiqin; Ahmed, Asma A.; Albert, Daniel H.; Bouska, Jennifer J.; Bousquet, Peter F.; Cunha, George A.; Glaser, Keith B.; Guo, Jun; Li, Junling; Marcotte, Patrick A.; Moskey, Maria D.; Pease, Lori J.; Stewart, Kent D.; Yates, Melinda; Davidsen, Steven K.; Michaelides, Michael R.
CORPORATE SOURCE: Global Pharmaceutical Research and Development, Abbott Laboratories, Abbott Park, IL, 60064-6100, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(16), 4326-4330
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:314939
GI



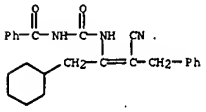
I

AB A series of isothiazolopyrimidines and isoxazolopyrimidines were synthesized and identified as potent KDR inhibitors. SAR studies led to isothiazolopyrimidine urea analogs that potently inhibit VEGFR tyrosine kinases (KDR enzymic and cellular IC50 values below 10 nM) as well as cKIT and TIE2. The selected compds. I [R = 3-MeC6H4, 2,5-F(Me)C6H3] display 56% and 48% oral bioavailability in mice, resp.
IT 909028-97-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isothiazolopyrimidines and isoxazolopyrimidines as multi-targeted inhibitors of receptor tyrosine kinases)
RN 909028-97-3 CAPLUS
CN 2-Butenethioamide, 3-amino-2-cyano-4-(4-nitrophenyl)- (CA INDEX NAME)

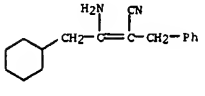


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:165963 CAPLUS
DOCUMENT NUMBER: 144:412131
TITLE: A high-yielding preparation of β-keto nitriles
AUTHOR(S): Ji, Yaohui; Trenkle, William C.; Vowles, James V.
CORPORATE SOURCE: Department of Chemistry, Brown University, Providence, RI, 02912, USA
SOURCE: Organic Letters (2006), 8(6), 1161-1163
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:412131
AB β-Keto nitriles are important precursors for a wide variety of biol. active heterocycles. A facile procedure for the high-yielding acylation of nitrile anions with unactivated esters to provide β-keto nitriles is reported. Thus, reaction of PhCH2CH2CN with PhCO2Et in THF containing EtCMe2OH K salt at room temperature for 10 min gave 95% PhCH2CH(CN)COPh. The procedure is successful with enolizable and nonenolizable esters as well as hindered nitrile anions.
IT 883854-15-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cyclization reaction of benzoyl isocyanate with aminoacrylonitrile derivative in preparation of keto nitriles via acylation of nitrile anions with unactivated esters)
RN 883854-15-7 CAPLUS
CN Benzamide, N-[[[2-cyano-1-(cyclohexylmethyl)-3-phenyl-1-propenyl]amino]carbonyl]- (9CI) (CA INDEX NAME)



IT 883854-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(heterocyclization of β-amino unsatd. nitrile in preparation of β-keto nitriles via acylation of nitrile anions with unactivated esters)
RN 883854-05-5 CAPLUS
CN Benzenepropanenitrile, α-(1-amino-2-cyclohexylethylidene)- (CA INDEX NAME)

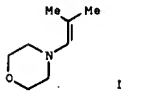


L15 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:128444 CAPLUS
DOCUMENT NUMBER: 144:369409
TITLE: Cyanamide in isocyanide-based MCRs
AUTHOR(S): Doemling, Alexander; Herdtweck, Eberhardt; Heck, Stefan
CORPORATE SOURCE: ABC Pharma, Munich, 81243, Germany
SOURCE: Tetrahedron Letters (2006), 47(11), 1745-1747
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369409
GI



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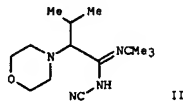
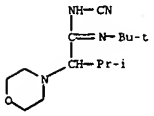


II

AB Cyanamide reacts with enamines and isocyanides in the presence of Lewis acids to give the hitherto unknown scaffold 2-amino-(N-cyano)-amidines. Preliminary scope and limitation of this novel reaction is described. E.g., reaction of enamine I, Me3CNC, and cyanamide in MeOH gave 65% 2-amino-(N-cyano)-amidine II.

IT 882006-90-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-amino-(N-cyano)-amidines by reaction of cyanamide with enamines and isocyanides)

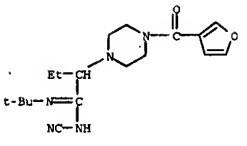
RN 882006-90-8 CAPLUS
CN 4-Morpholineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-(1-methylethyl)- (CA INDEX NAME)



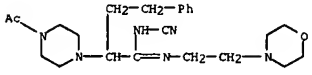
IT 882006-91-9P 882006-92-0P 882006-93-1P
882006-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-amino-(N-cyano)-amidines by reaction of cyanamide with enamines and isocyanides)

RN 882006-91-9 CAPLUS
CN 1-Piperazineethanimidamide, N-cyano-N'-(1,1-dimethylethyl)-α-ethyl-4-(3-furanylcarbonyl)- (CA INDEX NAME)

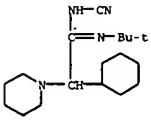
L15 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



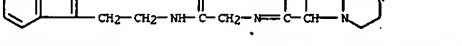
RN 882006-92-0 CAPLUS
CN 1-Piperazineethanimidamide, 4-acetyl-N-cyano-N'-[2-(4-morpholinyl)ethyl]-α-(2-phenylethyl)- (CA INDEX NAME)



RN 882006-93-1 CAPLUS
CN 1-Piperidineethanimidamide, N-cyano-α-cyclohexyl-N'-(1,1-dimethylethyl)- (CA INDEX NAME)



RN 882006-94-2 CAPLUS
CN Acetamide, 2-[[1-(cyanoamino)-4-phenyl-2-[4-(phenylmethyl)-1-piperazinyl]butylidene]amino]-N-[2-(1H-indol-3-yl)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:103473 CAPLUS
DOCUMENT NUMBER: 144:191975
TITLE: Preparation of aryl cyanoamidines as P2X7 antagonists for the treatment of pain, inflammation, and neurodegeneration.
INVENTOR(S): Carroll, William A.; Perez-Medrano, Arturo; Peddi, Sridhar; Florjancic, Alan S.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S. Pat. Appl. Publ., 30 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006025614	A1	20060202	US 2004-909502	20040802
US 7241776	B2	20070710		
WO 2006017406	A1	20060216	WO 2005-US27115	20050729
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2007232686	A1	20071004	US 2007-750633	20070518

PRIORITY APPLN. INFO.: US 2004-909502 A 20040802
OTHER SOURCE(S): CASREACT 144:191975; MARPAT 144:191975

AB Title compds. e.g. R2R1C(:NCN)NR6CHR3NR7COR4R5 [R1 = bond, alkylene, alkenylene, alkynylene; R2 = (substituted) aryl, heteroaryl; R3 = alkyl, haloalkyl; R4 = alkylene; R5 = halo, (substituted) aryl, heteroaryl; R6, R7 = H, alkyl], were prepared Thus, N-[1-(1H-1,2,3-benzotriazol-1-yl)-2,2-dimethylpropyl]-2-phenylacetamide (preparation given), N'-cyano-2-(2-methylphenyl)ethanimidamide (preparation given), and Cs2CO3 were stirred together for 10 h in MeCN to give N-[1-[(N-cyano-2-(2-methylphenyl)ethanimidoyl]amino]-2,2-dimethylpropyl]-2-phenylacetamide. Representative title compds. showed P2X7 antagonist activity with IC50 ≤10 μM.

IT 874993-05-2P 874993-06-3P 874993-07-4P
874993-08-5P 874993-09-6P 874993-10-9P
874993-11-0P 874993-12-1P 874993-13-2P
874993-14-3P 874993-15-4P 874993-16-5P
874993-18-7P 874993-19-8P 874993-20-1P
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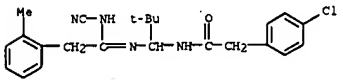
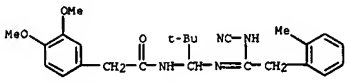
874993-51-8P 874993-52-9P 874993-53-0P

874993-54-1P 874993-55-2P 874993-56-3P
874993-57-4P 874993-58-5P 874993-59-6P
874993-60-9P 874993-61-0P 874993-62-1P
874993-63-2P 874993-64-3P 874993-65-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compd.; prepn. of aryl cyanoamidines as P2X7 antagonists for the treatment of pain, inflammation, and neurodegeneration)

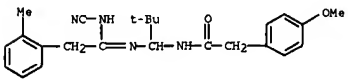
RN 874993-05-2 CAPLUS
CN Benzeneacetamide, 4-chloro-N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



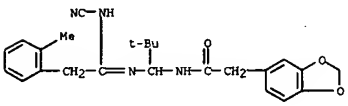
RN 874993-06-3 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-3,4-dimethoxy- (CA INDEX NAME)



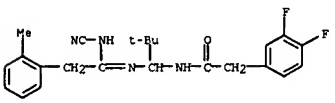
RN 874993-07-4 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-4-methoxy- (CA INDEX NAME)



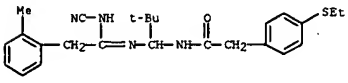
RN 874993-08-5 CAPLUS
CN 1,3-Benzodioxole-5-acetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



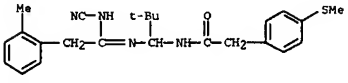
RN 874993-09-6 CAPLUS



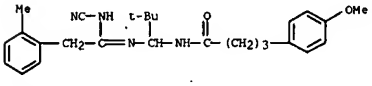
RN 874993-13-2 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-4-(ethylthio)- (CA INDEX NAME)



RN 874993-14-3 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-4-(methylthio)- (CA INDEX NAME)

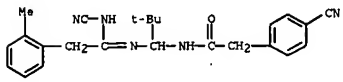


RN 874993-15-4 CAPLUS
CN Benzenebutanamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-4-methoxy- (CA INDEX NAME)

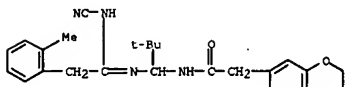


RN 874993-16-5 CAPLUS
CN Benzenepentanamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)

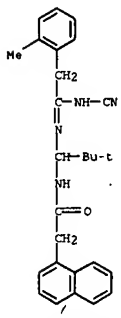
CN Benzeneacetamide, 4-cyano-N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



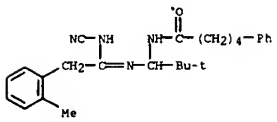
RN 874993-10-9 CAPLUS
CN 1,4-Benzodioxin-6-acetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-2,3-dihydro- (CA INDEX NAME)



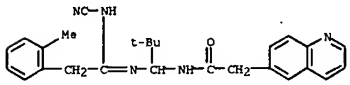
RN 874993-11-0 CAPLUS
CN 1-Naphthaleneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



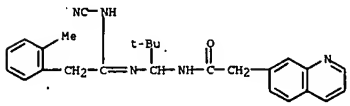
RN 874993-12-1 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-3,4-difluoro- (CA INDEX NAME)



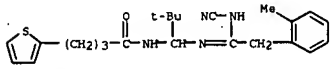
RN 874993-18-7 CAPLUS
CN 6-Quinolineacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



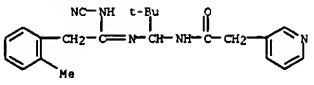
RN 874993-19-8 CAPLUS
CN 7-Quinolineacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



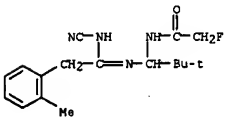
RN 874993-20-1 CAPLUS
CN 2-Thiophenebutanamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



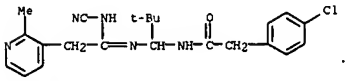
RN 874993-21-2 CAPLUS
CN 3-Pyridineacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



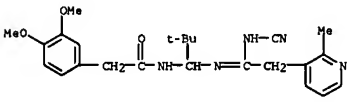
RN 874993-22-3 CAPLUS
CN Acetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]-2-fluoro- (CA INDEX NAME)



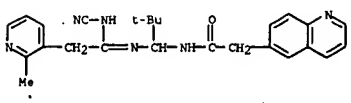
RN 874993-23-4 CAPLUS
CN Benzeneacetamide, 4-chloro-N-[1-[[1-(cyanoamino)-2-(2-methyl-3-pyridinyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



RN 874993-24-5 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methyl-3-pyridinyl)ethylidene]amino]-2,2-dimethylpropyl]-3,4-dimethoxy- (CA INDEX NAME)



RN 874993-25-6 CAPLUS
CN 6-Quinolineacetamide, N-[1-[[1-(cyanoamino)-2-(2-methyl-3-pyridinyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



RN 874993-26-7 CAPLUS
CN Benzeneacetamide, 4-chloro-N-[1-[[1-(cyanoamino)-2-(5-quinolinyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)

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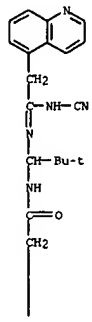

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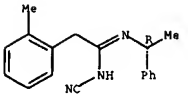
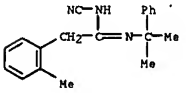
RN 874993-29-0 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[(1R)-1-phenylethyl]- (CA INDEX NAME)

Absolute stereochemistry.

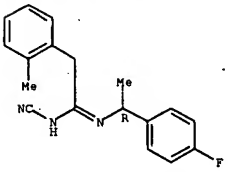


RN 874993-30-3 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-(1-methyl-1-phenylethyl)- (CA INDEX NAME)



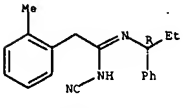
RN 874993-31-4 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[(1R)-1-(4-fluorophenyl)ethyl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 874993-32-5 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[(1R)-1-phenylpropyl]- (CA INDEX NAME)

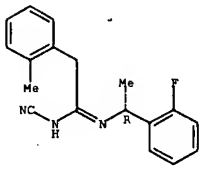
Absolute stereochemistry.



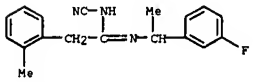
RN 874993-33-6 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[(1R)-1-(2-fluorophenyl)ethyl]-2-methyl-

(CA INDEX NAME)

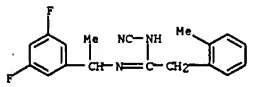
Absolute stereochemistry.



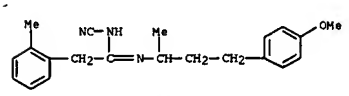
RN 874993-34-7 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[1-(3-fluorophenyl)ethyl]-2-methyl- (CA INDEX NAME)



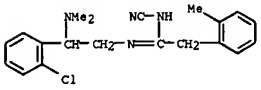
RN 874993-35-8 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[1-(3,5-difluorophenyl)ethyl]-2-methyl- (CA INDEX NAME)



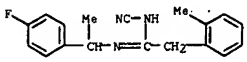
RN 874993-36-9 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[3-(4-methoxyphenyl)-1-methylpropyl]-2-methyl- (CA INDEX NAME)



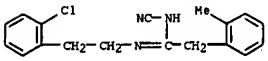
RN 874993-37-0 CAPLUS
CN Benzeneethanimidamide, N-[2-(2-chlorophenyl)-2-(dimethylamino)ethyl]-N'-cyano-2-methyl- (CA INDEX NAME)



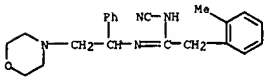
RN 874993-38-1 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[1-(4-fluorophenyl)ethyl]-2-methyl- (CA INDEX NAME)



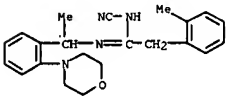
RN 874993-39-2 CAPLUS
CN Benzeneethanimidamide, N-[2-(2-chlorophenyl)ethyl]-N'-cyano-2-methyl- (CA INDEX NAME)



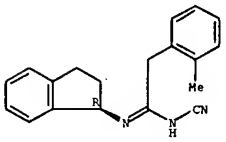
RN 874993-40-5 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[2-(4-morpholinyl)-1-phenylethyl]- (CA INDEX NAME)



RN 874993-41-6 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[1-[2-(4-morpholinyl)phenyl]ethyl]- (CA INDEX NAME)

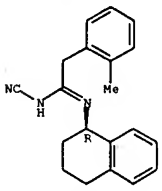


RN 874993-43-8 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[1-(3,5-difluorophenyl)ethyl]-2-(trifluoromethyl)- (CA INDEX NAME)

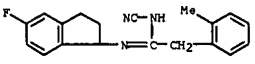


RN 874993-48-3 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[(1R)-1,2,3,4-tetrahydro-1-naphthalenyl]- (CA INDEX NAME)

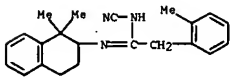
Absolute stereochemistry.



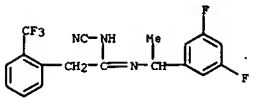
RN 874993-49-4 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-(5-fluoro-2,3-dihydro-1H-inden-1-yl)-2-methyl- (CA INDEX NAME)



RN 874993-50-7 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-(1,2,3,4-tetrahydro-1,1-dimethyl-2-naphthalenyl)- (CA INDEX NAME)

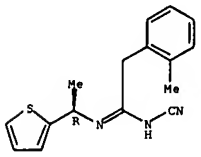


RN 874993-51-8 CAPLUS
CN Benzeneethanimidamide, N-(4-chloro-2,3-dihydro-1H-inden-1-yl)-N'-cyano-2-methyl- (CA INDEX NAME)

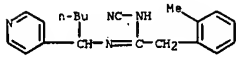


RN 874993-44-9 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[(1R)-1-(2-thienyl)ethyl]- (CA INDEX NAME)

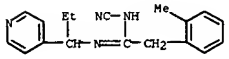
Absolute stereochemistry.



RN 874993-45-0 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[1-(4-pyridinyl)pentyl]- (CA INDEX NAME)

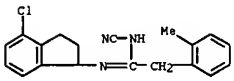


RN 874993-46-1 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[1-(4-pyridinyl)propyl]- (CA INDEX NAME)



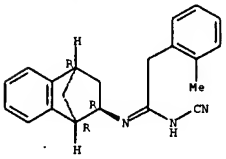
RN 874993-47-2 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[(1R)-2,3-dihydro-1H-inden-1-yl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.



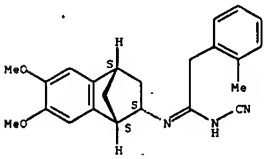
RN 874993-52-9 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[(1R,2R,4R)-1,2,3,4-tetrahydro-1,4-methanonaphthalen-2-yl]- (CA INDEX NAME)

Absolute stereochemistry.



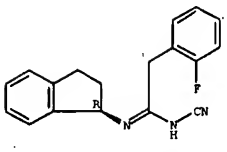
RN 874993-53-0 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[(1S,2S,4S)-1,2,3,4-tetrahydro-6,7-dimethoxy-1,4-methanonaphthalen-2-yl]- (CA INDEX NAME)

Absolute stereochemistry.

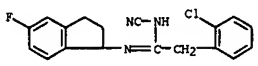


RN 874993-54-1 CAPLUS
CN Benzeneethanimidamide, N-cyano-N'-[(1R)-2,3-dihydro-1H-inden-1-yl]-2-fluoro- (CA INDEX NAME)

Absolute stereochemistry.

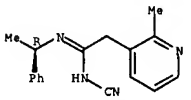


RN 874993-55-2 CAPLUS
CN Benzeneethanimidamide, 2-chloro-N-cyano-N'-(5-fluoro-2,3-dihydro-1H-inden-1-yl)- (CA INDEX NAME)

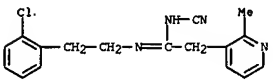


RN 874993-56-3 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-2-methyl-N'-[(1R)-1-phenylethyl]- (CA INDEX NAME)

Absolute stereochemistry.

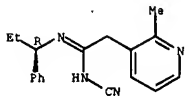


RN 874993-57-4 CAPLUS
CN 3-Pyridineethanimidamide, N-[2-(2-chlorophenyl)ethyl]-N'-cyano-2-methyl- (CA INDEX NAME)

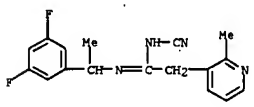


RN 874993-58-5 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-2-methyl-N'-[(1R)-1-phenylpropyl]- (CA INDEX NAME)

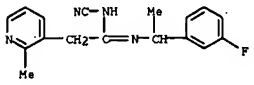
Absolute stereochemistry.



RN 874993-59-6 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-N'-[1-(3,5-difluorophenyl)ethyl]-2-methyl- (CA INDEX NAME)

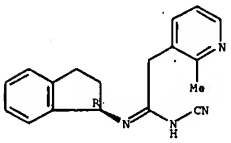


RN 874993-60-9 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-N'-[1-(3-fluorophenyl)ethyl]-2-methyl- (CA INDEX NAME)

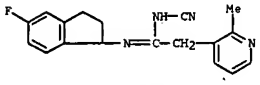


RN 874993-61-0 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-N'-[(1R)-2,3-dihydro-1H-inden-1-yl]-2-methyl- (CA INDEX NAME)

Absolute stereochemistry.

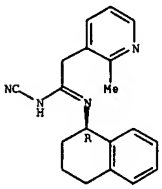


RN 874993-62-1 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-N'-(5-fluoro-2,3-dihydro-1H-inden-1-yl)-2-methyl- (CA INDEX NAME)



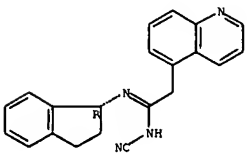
RN 874993-63-2 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-2-methyl-N'-[(1R)-1,2,3,4-tetrahydro-1-naphthalenyl]- (CA INDEX NAME)

Absolute stereochemistry.



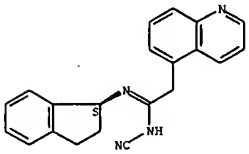
RN 874993-64-3 CAPLUS
CN 5-Quinolineethanimidamide, N-cyano-N'-[(1R)-2,3-dihydro-1H-inden-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.



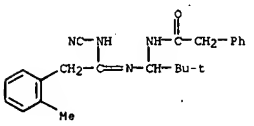
RN 874993-65-4 CAPLUS
CN 5-Quinolineethanimidamide, N-cyano-N'-[(1S)-2,3-dihydro-1H-inden-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.

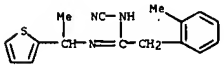


IT 874993-66-5P 874993-87-0P 874993-88-1P
874993-89-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryl cyanoamidines as P2X7 antagonists for the treatment of
pain, inflammation, and neurodegeneration)

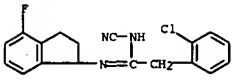
RN 874993-66-5 CAPLUS
CN Benzeneacetamide, N-[1-[[1-(cyanoamino)-2-(2-methylphenyl)ethylidene]amino]-2,2-dimethylpropyl]- (CA INDEX NAME)



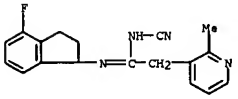
RN 874993-87-0 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl-N'-[1-(2-thienyl)ethyl]- (CA INDEX NAME)



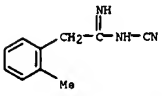
RN 874993-88-1 CAPLUS
CN Benzeneethanimidamide, 2-chloro-N-cyano-N'-(4-fluoro-2,3-dihydro-1H-inden-1-yl)- (CA INDEX NAME)



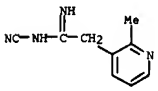
RN 874993-89-2 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-N'-(4-fluoro-2,3-dihydro-1H-inden-1-yl)-2-methyl- (CA INDEX NAME)



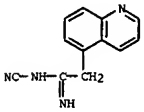
IT 874993-68-7P 874993-73-4P 874993-75-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl cyanoamidines as P2X7 antagonists for the treatment of
pain, inflammation, and neurodegeneration)
RN 874993-68-7 CAPLUS
CN Benzeneethanimidamide, N-cyano-2-methyl- (CA INDEX NAME)



RN 874993-73-4 CAPLUS
CN 3-Pyridineethanimidamide, N-cyano-2-methyl- (CA INDEX NAME)



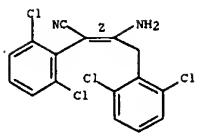
RN 874993-75-6 CAPLUS
CN 5-Quinolineethanimidamide, N-cyano- (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS

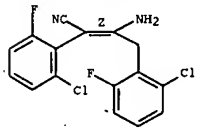
ACCESSION NUMBER: 2005:1094893 CAPLUS
DOCUMENT NUMBER: 144:31624
TITLE: Double-Stranded Metal-Organic Networks for One-Dimensional Mixed Valence Coordination Polymers
AUTHOR(S): Robertson, Daniel; Cannon, John F.; Gerasimchuk, Nikolay
CORPORATE SOURCE: Department of Chemistry, Southwest Missouri State University, Springfield, MO, 65804, USA
SOURCE: Inorganic Chemistry (2005), 44(23), 8326-8342
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:31624
AB The design of new types of metal-organic networks and the search for unusual crystal architecture represents an important task for modern inorg. and materials chemical research. A group of new monosubstituted phenylcyanoximes, containing F, Cl, and Br atoms at the 2, 3, or 4 positions, were synthesized using the high yield nitrosation reaction with CH3-ONO and were spectroscopically (1H NMR, 13C NMR, UV-visible, IR, mass spectrometry) and structurally characterized. Results of x-ray anal. revealed nonplanar trans-anti geometry for 2-chlorophenyl(oximino)acetonitrile, H(2Cl-PhCO); a nonplanar anti configuration for 4-chlorophenyl(oximino)acetonitrile, H(4Cl-PhCO); and planar cis-syn geometry for 3-fluorophenyl(oximino)acetonitrile, H(3F-PhCO). All arylcyanoximes undergo deprotonation in solns. with the formation of colored anions exhibiting pronounced neg. solvatochromism in polar protic and aprotic solvents. Nine Tl(I) cyanoximates were obtained using the reaction between hot (.apprx.95°) aqueous solns. of Tl2CO3 and solid powdery monohalogenated arylcyanoximes HL. Crystal structures of two Tl(I) cyanoximates [Tl(2Cl-PhCO) and Tl(4Br-PhCO)] contained centrosym. dimeric units (TlL)2 that are connected to a coordination polymer by an O atom of the oxime group of the neighboring mol. Cyanoxime anions act as bridging ligands in both structures where the polymeric motif consists of double-stranded Tl-O chains interconnected with the formation of zigzagging Tl2O2 planar rhombes. Tl atoms form infinite linear arrays with close intermetallic sepns. The nearest Tl(I)···Tl(I) distances are 3.838 and 4.058 Å in the Tl(2Cl-PhCO) and Tl(4Br-PhCO) structures, resp., close to that in metallic Tl (3.456 Å). Monosubstituted Ph groups are well aligned in π-stacking columns that are perpendicular to the array of Tl(I) atoms and stabilize formed structures. Coordination polyhedrons of Tl(I) in these complexes represent distorted trigonal pyramids with stereoactive lone pair.
IT 870619-97-9 870619-99-1
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(Thorpe condensation product from attempted nitrosation of dihalophenylacetonitrile with poor quality alkyl nitrite)
RN 870619-97-9 CAPLUS
CN Benzeneacetonitrile, α-[1-amino-2-(2,6-dichlorophenyl)ethylidene]-2,6-dichloro-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 870619-99-1 CAPLUS
CN Benzeneacetonitrile, α-[1-amino-2-(2-chloro-6-fluorophenyl)ethylidene]-2-chloro-6-fluoro-, (αZ)- (CA INDEX NAME)

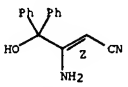
Double bond geometry as shown.



REFERENCE COUNT: 184 THERE ARE 184 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:359325 CAPLUS
DOCUMENT NUMBER: 144:88091
TITLE: Cyanoacetylene and its derivatives. Part XXXII. Addition of ammonia and methylamine to 4-hydroxy-4,4-diphenyl-2-butynenitrile
AUTHOR(S): Mal'kina, A. G.; Sokolyanskaya, L. V.; Kudyakova, R. N.; Sinegovskaya, L. M.; Albanov, A. I.; Shemyakina, O. A.; Trofimov, B. A.
CORPORATE SOURCE: Favorskii Irkutsk Institute of Chemistry, Siberian Division, Russian Academy of Sciences, Irkutsk, 664033, Russia
SOURCE: Russian Journal of Organic Chemistry (2005), 41(1), 61-66
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: Pleiades Publishing, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:88091
AB Nucleophilic addition of 25% aqueous NH3 and MeNH2 to 4-hydroxy-4,4-diphenyl-2-butynenitrile occurs under mild conditions to afford 4-amino- or 4-methylamino-2,5-dihydro-5,5-diphenyl-2-iminofurans. 4-Hydroxy-4,4-diphenyl-2-butynenitrile in anhydrous liquid NH3 gives rise to 3-amino-4-hydroxy-4,4-diphenyl-2-butenenitrile which is quant. converted into the corresponding iminodihydrofuran or iminodihydrofuran.HCl in the presence of 10 wt% of KOH or gaseous HCl. 4-Amino- and 4-methylamino-2-iminofurans react with 4-hydroxy-4-methyl-2-pentynenitrile to give 3-(4-amino- and 4-methylamino-5,5-diphenyl-2,5-dihydrofuran-2-ylideneamino)-4-hydroxy-4-methyl-2-pentenenitriles.
IT 872494-14-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of iminodihydrofurans by addition of ammonia and methylamine to hydroxydiphenylbutynenitrile)
RN 872494-14-9 CAPLUS
CN 2-Butenenitrile, 3-amino-4-hydroxy-4,4-diphenyl-, (2Z)- (CA INDEX NAME)

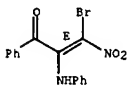
Double bond geometry as shown.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:892690 CAPLUS
DOCUMENT NUMBER: 142:392133
TITLE: Preparation of 2-benzoyl-1-bromo-1-nitroethene
AUTHOR(S): Sadikov, K. D.; Litovchenko, K. M.; Makarenko, S. V.; Berestovitskaya, V. M.
CORPORATE SOURCE: Herzen Russian State Pedagogical University, St. Petersburg, 191186, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2004), 40(8), 1219-1220
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:392133
AB 2-Benzoyl-1-bromo-1-nitroethene (I) is prepared in 2 stages: bromination of 2-benzoyl-1-nitroethene (II) and subsequent dehydrobromination of the addition product, 2-benzoyl-1,2-dibromo-1-nitroethene (III). The reaction of II with a double excess of Br in glacial acetic acid or CCl4 afforded the dibromide III. Yield was best (65%) in CCl4. Dehydrohalogenation of III in CCl4 was conducted with Et3N within 1 h at room temperature Compound I was isolated in 63% yield as light-yellow crystals (mp. 25-26°). Nitroenamine was also prepared directly from dibromide III or I by reaction with aniline.
IT 849729-61-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-benzoyl-1-bromo-1-nitroethene and 2-anilino-2-benzoyl-1-nitroethene)
RN 849729-61-9 CAPLUS
CN 2-Propen-1-one, 3-bromo-3-nitro-1-phenyl-2-(phenylamino)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

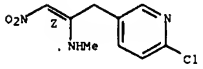
L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:566527 CAPLUS
DOCUMENT NUMBER: 141:101553
TITLE: Preparation of insecticidal, acaricidal and nematocidal pyridine derivatives
INVENTOR(S): Benko, Zoltan Laszlo; Deamicis, Carl Vincent; Demeter, David Anthony; Markley, Lowell Dean; Samaritoni, Jack Geno; Schmidt, Carrie Lynn Rau; Zhu, Yuamning; Erickson, W. Randal; Anzeveno, Peter Biagio; Pechacek, James Todd; Watson, Gerald Bryan; Deboer, Gerrit Jan; Sheets, Joel Jay; Zabik, Susan Erhardt; Yerkes, Carla Nanette; Schobert, Christian Thomas; Dripps, James Edwin; Dintenfass, Leonard Paul; Karr, Laura Lee; Neese, Paul Allen; Huang, Jim Xinpei; Gifford, James Michael
PATENT ASSIGNEE(S): Dow Agrosciences LLC, USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004057960	A2	20040715	WO 2003-US41067	20031219
WO 2004057960	A3	20041104		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003303336	A1	20040722	AU 2003-303336	20031219
EP 1572656	A2	20050914	EP 2003-808550	20031219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006063741	A1	20060323	US 2005-535653	20050519
PRIORITY APPLN. INFO.:			US 2002-435928P	P 20021220
			WO 2003-US41067	W 20031219

OTHER SOURCE(S): MARPAT 141:101553
AB The compds. QCR1R2C(:XZ)NR3R4 [Q = carbocyclyl or heterocyclyl, preferably pyridyl; X = N, CR, COR, CSOnR; CNR2, etc.; R1-5 = (cyclo)alkyl, (cyclo)alkenyl, alkoxy, aryl, etc.; n = 0, 1 or 2; Z = CN or NO2; R1CR2 = carbocyclyl or heterocyclyl] are prepared as insecticide, acaricide or nematocides.
IT 717106-20-2P 717106-21-3P 717106-22-4P
717106-23-5P 717106-24-6P 717106-25-7P
717106-26-8P 717106-27-9P 717106-28-0P
717106-29-1P 717106-30-4P 717106-31-5P
717106-32-6P 717106-33-7P 717106-34-8P
717106-35-9P 717106-36-0P 717106-37-1P
717106-38-2P 717106-39-3P 717106-40-6P
717106-41-7P 717106-42-8P 717106-43-9P
717106-44-0P 717106-45-1P 717106-46-2P
717106-47-3P 717106-48-4P 717106-49-5P
717106-50-8P 717106-51-9P 717106-52-0P

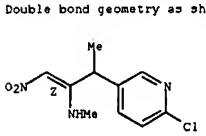
L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
717106-53-1P 717106-54-2P 717106-55-3P
717106-56-4P 717106-57-5P 717106-58-6P
717106-60-0P 717106-61-1P 717106-62-2P
717106-63-3P 717106-64-4P 717106-65-5P
717106-67-7P 717106-68-8P 717913-04-7P
717913-05-8P
RL: AGR (Agricultural use); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. as insecticide, acaricide and nematocides)
RN 717106-20-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



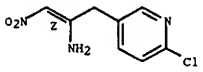
RN 717106-21-3 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N,β-dimethyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



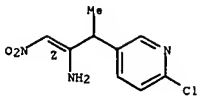
RN 717106-22-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



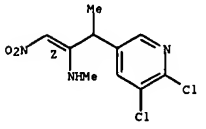
RN 717106-23-5 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



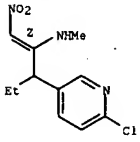
RN 717106-24-6 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-N,β-dimethyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



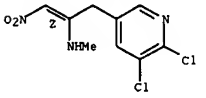
RN 717106-25-7 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-ethyl-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



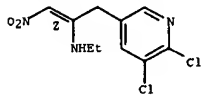
RN 717106-26-8 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



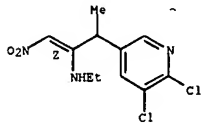
RN 717106-27-9 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-N-ethyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



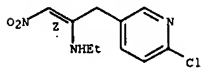
RN 717106-28-0 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-N-ethyl-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



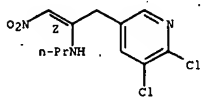
RN 717106-29-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-ethyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



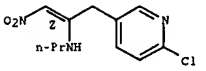
RN 717106-30-4 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-α-(nitromethylene)-N-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



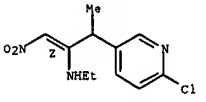
RN 717106-31-5 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-N-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



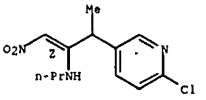
RN 717106-32-6 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-ethyl-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



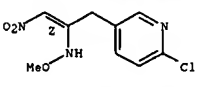
RN 717106-33-7 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



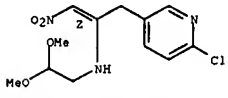
RN 717106-34-8 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methoxy-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



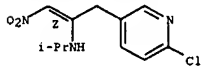
RN 717106-35-9 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(2,2-dimethoxyethyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



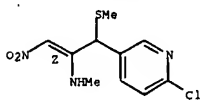
RN 717106-36-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(1-methylethyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



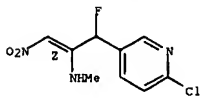
RN 717106-37-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-β-(methylthio)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



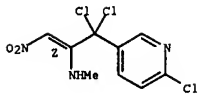
RN 717106-38-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-fluoro-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



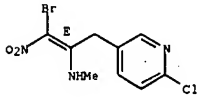
RN 717106-39-3 CAPLUS
CN 3-Pyridineethanamine, β,β,6-trichloro-N-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



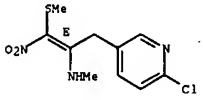
RN 717106-40-6 CAPLUS
CN 3-Pyridineethanamine, α-(bromonitromethylene)-6-chloro-N-methyl-, (αE)- (CA INDEX NAME)

Double bond geometry as shown.



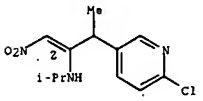
RN 717106-41-7 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-[(methylthio)nitromethylene]-, (αE)- (CA INDEX NAME)

Double bond geometry as shown.



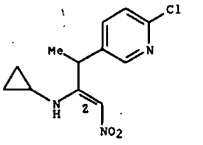
RN 717106-42-8 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(1-methylethyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



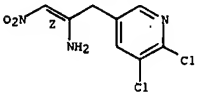
RN 717106-43-9 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-N-(phenylmethyl)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



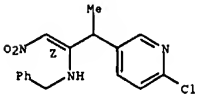
RN 717106-47-3 CAPLUS
CN 3-Pyridineethanamine, 5,6-dichloro-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



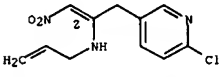
RN 717106-48-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-(phenylmethyl)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

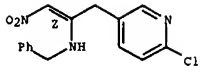


RN 717106-49-5 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-N-2-propenyl-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

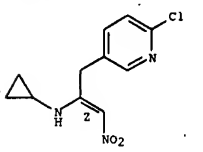


RN 717106-50-8 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(2-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)



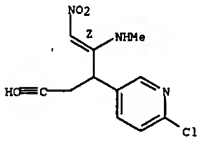
RN 717106-44-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-cyclopropyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



RN 717106-45-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-2-propynyl-, (αZ)- (9CI) (CA INDEX NAME)

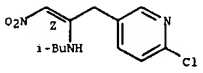
Double bond geometry as shown.



RN 717106-46-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-cyclopropyl-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

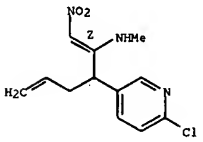
Double bond geometry as shown.

Double bond geometry as shown.



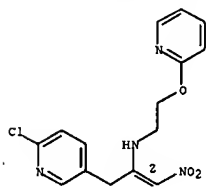
RN 717106-51-9 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-2-propenyl-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



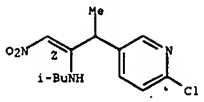
RN 717106-52-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-N-[2-(2-pyridinyloxy)ethyl]-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



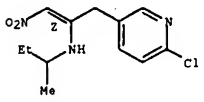
RN 717106-53-1 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(2-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



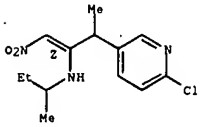
RN 717106-54-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(1-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



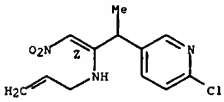
RN 717106-55-3 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-N-(1-methylpropyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



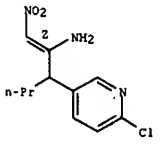
RN 717106-56-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-2-propenyl-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



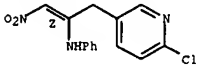
RN 717106-57-5 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-β-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



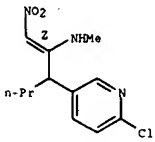
RN 717106-58-6 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-α-(nitromethylene)-N-phenyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



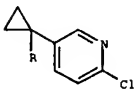
RN 717106-60-0 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-methyl-α-(nitromethylene)-β-propyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



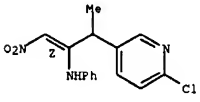
RN 717106-61-1 CAPLUS
CN Cyclopropanemethanamine, 1-(6-chloro-3-pyridinyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



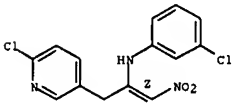
RN 717106-62-2 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-β-methyl-α-(nitromethylene)-N-phenyl-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



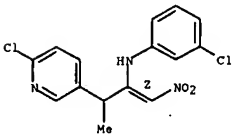
RN 717106-63-3 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(3-chlorophenyl)-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



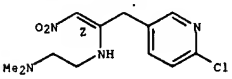
RN 717106-64-4 CAPLUS
CN 3-Pyridineethanamine, 6-chloro-N-(3-chlorophenyl)-β-methyl-α-(nitromethylene)-, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.



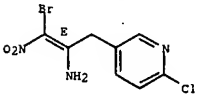
RN 717106-65-5 CAPLUS
CN 1,2-Ethanediamine, N'-[(1Z)-1-[(6-chloro-3-pyridinyl)methyl]-2-nitroethenyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



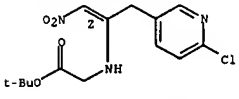
RN 717106-67-7 CAPLUS
CN 3-Pyridineethanamine, α-(bromonitromethylene)-6-chloro-, (αE)- (CA INDEX NAME)

Double bond geometry as shown.



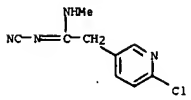
RN 717106-68-8 CAPLUS
CN Glycine, N-[(1Z)-1-[(6-chloro-3-pyridinyl)methyl]-2-nitroethenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Double bond geometry as shown.

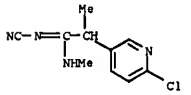


RN 717913-04-7 CAPLUS
CN 3-Pyridineethanimidamide, 6-chloro-N'-cyano-N-methyl-, [C(Z)]- (9CI) (CA INDEX NAME)

L15 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 717913-05-8 CAPLUS
CN 3-Pyridineethanimidamide, 6-chloro-N'-cyano-N,α-dimethyl-, [C(Z)]-(9CI) (CA INDEX NAME)



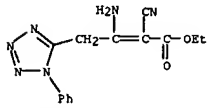
L15 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:204642 CAPLUS
DOCUMENT NUMBER: 142:56200
TITLE: Product class 30: tetrazoles
AUTHOR(S): Brigas, A. F.
CORPORATE SOURCE: Universidade Algarve UCEH, Faro, 8000, Port.
SOURCE: Science of Synthesis (2004), 13, 861-915
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review. Methods of preparing tetrazoles are reviewed including cyclization, ring transformation, aromatization, and substituent modification.

IT 803739-53-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tetrazoles via cyclization, ring transformation, aromatization, and substituent modification)

RN 803739-53-9 CAPLUS
CN 2-Butenoic acid, 3-amino-2-cyano-4-(1-phenyl-1H-tetrazol-5-yl)-, ethyl ester (CA INDEX NAME)



REFERENCE COUNT: 307 THERE ARE 307 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1932:11638 CAPLUS
DOCUMENT NUMBER: 26:11638
ORIGINAL REFERENCE NO.: 26:1239f-i,1240a-f
TITLE: Ketimide-enamine tautomerism. III. Chemical and spectrochemical methods of determining structure
AUTHOR(S): v. Auwers, K.; Wunderling, H.
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1931), 64B, 2758-67
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB The starting materials in the long series of Thorpe's investigations on substances capable of ketimide-enamine tautomerism were various cyano compds. which under the influence of Na alcoholates condense with themselves or with other substances, generally with formation of open-chain compds. which can subsequently be converted into cyclic compds. by means of concentrated H2SO4. Thus, from NCCHNaCO2Et and PhCH2CN was obtained Et 1,3-diamino-2-naphthoate (I) to which, because of its golden yellow color, T. assigned the diimide structure (II), while to the colorless acid he gave the diamino, structure (H2N)2C10H5CO2H. He assumed a similar difference between the "yellow" ester (III) of 1,3-dihydroxy-2-naphthoic acid (IV) and the "colorless" acid (Metzner, the discoverer of these compds., describes both as being "yellowish"). In view of the ease with which hydroaromatic change into aromatic compds. whenever possible, v. A. and W. undertook to determine the structure of I and III spectrochemically. Ketones of the type PhCOAlk normally show ΣΣRefr. about 0.5 and ΣΣDisp. 28% and when they are converted by ring closure into α-tetralone-like compds. these values increase somewhat (e. g., 0.73 and 40%, resp., for α-tetralone itself). III, if it had the diketone structure, should show exaltations of a similar order of magnitude (at least, they should not exceed 1.0 and 50%), but detns. made in α-C10H7Me gave values for ΣΣ of 3.07, 3.37 and 213% for α, D and β-α when calculated on the basis of the diketone structure, and 2.24, 2.51, 169% on the basis of the di-HO structure; the latter values agree well with those of Krollpfeiffer on C10H8 derivs. The free acid could not be studied because of its low solubility in all suitable solvents. Similarly, from observations of Moureu and Mignonac, ΣΣ for imides of the type PhC(:NH)Alk is 0.5, and diimides of type II might be expected to show an exaltation of 0.75 or 1.0 at most, whereas the values actually obtained, when calculated on the basis of such a structure, were 3.99, 4.42 and 170% for α, D and β-α, resp. On the other hand, the values calculated on the basis of the diamino structure (3.14, 3.54, 133%) agree well with those for mono- and di-amino derivs. of C10H8. Thorpe grouped his compds. into 3 classes: (1) imilles with "short amine phase" (2) pronouncedly tautomeric compds.; (3) amines with "short imine phase." The nature of the individual compds., according to him, was determined by the nature and number of "negative" substituents (CN, CO2R, CO2H, Ph), the position of the NH2 or NH groups with respect to these substituents, and certain steric factors. He based his classification on the behavior of the compds. towards acids, especially HCl; imines are hardly basic, do not dissolve in concentrated HCl and on heating are rapidly and completely hydrolyzed to the ketones; amines form salts and are not hydrolyzed even on long heating with acids; compds. of class (2) dissolve in HCl, the rapidity and extent to which the resulting salts are converted back into the amine or hydrolyzed to the ketones by water indicating the position of the equilibrium imine .dblarw. amine. There are many objections to the Thorpe

L15 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

theory in individual cases, and v. A. and W. believe there is no need of assuming amine and imine forms to explain the differing behavior of these N compds. As is so often the case in tautomerism problems, purely chem. methods here also do not suffice to furnish a soln. To solve the problem spectro-chemically it was necessary first to study some unsatd. amino nitriles, and measurements were accordingly made on diacetonitrile (V), dipropionitrile (VI), Et α-cyano-β-amino-γ-phenylcrotonate (VII), β-aminocinnamonitrile (VIII), β-diethylaminocinnamonitrile (IX) and Et β-diethylaminocinnamate (X). These showed that the earlier detns. on V were for some reason wrong and that enamine-nitriles have greater, not smaller, exaltations than the enamine-esters. VIII-X, from their ΣΣ values, are true cinnamic derivs. The high exaltations of 2-amino-1-cyanoindene (XI), considered by Thorpe to be 2-imino-1-cyanohydrindene, are not reconcilable with the imine structure. This was confirmed by measurements on 1-cyano-β-hydrindone (XII) and its O- (XIII) and N-Me ethers (XIV). v. A. and W. conclude that Thorpe's classification has no basis in fact and that the substances studied by him are all enamines. Of course, spectro-chemistry, in this as in other fields, has its limitations and whether these enamines are homogeneous or admixed with certain quantities of the tautomeric ketimines must, in general, be left an open question. Values for d4t, n for α, He and β at t° and EM for α, D and β-α for I-X and also for di-Et 1-aminoglutaconate are given.

IT 859179-72-9P, Crotonic acid, β-amino-α-cyano-γ-phenyl-, ethyl ester
RL: PREP (Preparation)
(preparation of)

RN 859179-72-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED